

CONFIDENCE BOUNDS FOR THE SENSITIVITY LACK OF A LESS SPECIFIC DIAGNOSTIC TEST, WITHOUT GOLD STANDARD

BY LUTZ MATTNER AND FRAUKE MATTNER

Universität Trier and Kliniken der Stadt Köln

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We consider the problem of comparing two diagnostic tests based on a sample of paired test results without true state determinations, in cases where the second test can reasonably be assumed to be at least as specific as the first. For such cases, we provide two informative confidence bounds: A lower one for the prevalence times the sensitivity gain of the second test with respect to the first, and an upper one for the sensitivity of the first test. Neither conditional independence of the two tests nor perfectness of any of them needs to be assumed.

An application of the proposed confidence bounds to a sample of 256 pairs of laboratory test results for toxigenic Clostridium difficile provides evidence for a dramatic sensitivity gain through first appropriately culturing Clostridium difficile from stool samples before applying an enzyme-immuno-assay.

Dedicated to Abram M. Kagan on the occasion of AMISTAT 2011 at Prague

1. Main results and applications.

1.1. *Introduction and outline.* Inference for sensitivities or specificities of diagnostic tests can be next to impossible if no suitable method for determining true states is available. Motivated by a real data problem described below, and in more detail in [6, 7], we consider here the situation where paired observations for two tests are given and where it can be assumed that the first test is less specific than the second. Can we then infer from suitable observations that the second test is more sensitive, and hence better, than the first? And if yes, by how much?

Theorem 1.1 in Subsection 1.6 below provides a simple and in some sense optimal answer. The necessary notation and concepts are carefully explained

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before in Subsections 1.2-1.4, but some readers may wish to start less formally by first consulting Subsection 1.5, which introduces our motivating example, and then proceed to the application of Theorem 1.1 given immediately after its statement. There it turns out that the answer to the above “how much?” question depends on upper bounds assumed for the prevalence, but that nevertheless interesting upper bounds for the sensitivity of the first test can be given without such an assumption, using our Theorems 1.2 and 1.3. Neither of our results uses any further assumptions, such as the conditional independence assumption as discussed and criticized, for example, in [8, Section 7.3].

We prove Theorems 1.1-1.3 in the final Section 4, after collecting auxiliary results on latent class models in Section 2 and proving them in Section 3.

While there is a substantial literature on various aspects of the statistics of diagnostic tests, see in particular the monographs [1, 8, 11], we are not aware of a previous treatment of the problem considered here. Our assumption that the first test is less specific than the second may seem very special, so let us point out that, for the purpose of obtaining upper bounds on the sensitivity of the first test, our assumption may by Theorem 1.3 replace the always less plausible assumption of perfectness of the second test, see Subsection 1.8 for an example.

1.2. Mathematical and probabilistic notation and conventions. We use “iff” as an abbreviation for “if and only if”. We write $\mathbb{N} := \{1, 2, 3, \dots\}$, $\mathbb{N}_0 := \{0\} \cup \mathbb{N}$, and $\bar{\mathbb{R}} := \mathbb{R} \cup \{-\infty, \infty\}$. We put $x/0 := \infty$ for $x > 0$, but we define $0/0$ below at each occurrence separately to be either 0 or $1/2$ or 1. A subscript “+” indicates summation with respect to the variable it replaces, as in $x_+ = \sum_{i=1}^n x_i$ for $x \in \mathbb{R}^n$ or in (6) below for $k \in \mathbb{N}_0^{\{0,1\}^2}$. By contrast, a superscript “+” indicates the positive part, so $x^+ = x \vee 0 = \max\{x, 0\}$ and correspondingly $x^- = (-x) \vee 0$ for $x \in \bar{\mathbb{R}}$. As usual, the order theoretic operations \wedge and \vee are computed first in expressions like $a b \wedge c := a (b \wedge c) = a \min\{b, c\}$.

If \mathcal{X} and \mathcal{Y} are any sets, then

$$\begin{aligned} \text{prob}(\mathcal{X}) &:= \left\{ (\mathcal{X} \ni x \mapsto p_x \in [0, 1]) : \sum_{x \in \mathcal{X}} p_x = 1 \right\} \\ \text{mark}(\mathcal{X}, \mathcal{Y}) &:= \left\{ (\mathcal{X} \times \mathcal{Y} \ni (x, y) \mapsto p_{y|x}) : p_{\cdot|x} \in \text{prob}(\mathcal{Y}) \text{ for } x \in \mathcal{X} \right\} \end{aligned}$$

denote the set of all discrete probability densities on \mathcal{X} and the set of all discrete Markov transition densities from \mathcal{X} to \mathcal{Y} , where the standard dot notation $p_{\cdot|x}$ for the partial function $y \mapsto p_{y|x}$ has been used. With $M_{n,p}$ we denote the multinomial distribution with sample size parameter n and success probability vector $p \in \text{prob}(\mathcal{X})$ for some \mathcal{X} , that is, $M_{n,p}(\{k\}) = n! \prod_{x \in \mathcal{X}} (p_x^{k_x} / k_x!)$ for $k \in \mathbb{N}_0^{\mathcal{X}}$ with $\sum_{x \in \mathcal{X}} k_x = n$.

1.3. *Confidence bounds and their comparison.* Let $\mathcal{P} = (P_\vartheta : \vartheta \in \Theta)$ be a statistical model on a sample space \mathcal{X} and let $\kappa : \Theta \rightarrow \overline{\mathbb{R}}$ be a parameter of interest. We allow nonidentifiability of κ , that is, we may have $\vartheta_1, \vartheta_2 \in \Theta$ with $P_{\vartheta_1} = P_{\vartheta_2}$ but $\kappa(\vartheta_1) \neq \kappa(\vartheta_2)$. For lack of any better name, let us call the pair (\mathcal{P}, κ) an *estimation problem*. Let $\beta \in [0, 1]$. Then every measurable function $\underline{\kappa} : \mathcal{X} \rightarrow \overline{\mathbb{R}}$ with $P_\vartheta(\underline{\kappa} \leq \kappa(\vartheta)) \geq \beta$ for every $\vartheta \in \Theta$ is called a *lower β -confidence bound* for (\mathcal{P}, κ) .

Now let $\underline{\kappa}$ and $\tilde{\kappa}$ be both lower β -confidence bounds for (\mathcal{P}, κ) . Then everybody seems to agree that for preferring $\underline{\kappa}$ over $\tilde{\kappa}$, it would be desirable to have

$$(1) \quad P_\vartheta(\tilde{\kappa} \geq t) \leq P_\vartheta(\underline{\kappa} \geq t) \quad \text{for } \vartheta \in \Theta \text{ and } t < \kappa(\vartheta)$$

For example, Lehmann and Romano [3, page 72] would call $\underline{\kappa}$ *uniformly most accurate* if (1) held for every $\tilde{\kappa}$ as above, but such a $\underline{\kappa}$ is known to exist in exceptional cases only. The desideratum (1) could be supplemented by conditions for $t \geq \kappa(\vartheta)$ in different ways, see [9, page 162] for one possibility, but we stick to (1) as it is. Thus we call $\tilde{\kappa}$ *worse* than $\underline{\kappa}$, and equivalently $\underline{\kappa}$ *better* than $\tilde{\kappa}$, if (1) holds, and *strictly so*, if in addition strict inequality holds in (1) for at least one ϑ and one t . Accordingly, $\underline{\kappa}$ is called *admissible* as a β -confidence bound for (\mathcal{P}, κ) , if no other such bound $\tilde{\kappa}$ is strictly better. Finally, $\underline{\kappa}$ and $\tilde{\kappa}$ are called *equivalent*, if each is worse than the other, that is, if (1) holds with “=” in place of “ \leq ”.

1.4. *Latent class models for diagnostic tests.* Informally speaking, a (di-chotomous) diagnostic test is a procedure yielding a guess $\in \{0, 1\}$ for the state $\in \{0, 1\}$ of any item belonging to some specified population. In this context, 0 is called *negative* and 1 is called *positive*. In medicine, the population often consists of persons, for whom a positive state means actually having a certain disease, and a positive diagnosis means to be guessed to have the disease. The accuracy of a diagnostic test is modelled by two numbers called *specificity* and *sensitivity*, with specificity interpreted as the probability that a random negative item is diagnosed as negative, and sensitivity as the probability that a random positive item is diagnosed as positive. The probability of diagnosing a random item from the whole population as positive, say, then of course depends also on the *prevalence*, which is the probability of such an item to be actually positive. If we formalize the above, for samples of size n rather than 1, and also admitting more generally d tests, rather than just

one, to be applied to every item, we arrive at the following model considered in essence already in [2].

Let $d \in \mathbb{N}$ and

$$\Theta_d := \text{prob}(\{0, 1\}) \times \text{mark}(\{0, 1\}, \{0, 1\}^d)$$

For $\vartheta = (\pi, \chi) \in \Theta_d$, let $\mu(\vartheta) \in \text{prob}(\{0, 1\}^d)$ denote the second marginal of the density

$$(2) \quad \{0, 1\} \times \{0, 1\}^d \ni (i, j) \mapsto \pi_i \chi_{j|i}$$

so that

$$(3) \quad \left(\mu(\vartheta) \right)_j = \sum_{i=0}^1 \pi_i \chi_{j|i} \quad \text{for } j \in \{0, 1\}^d \text{ and } \vartheta \in \Theta_d$$

Finally, with a given $n \in \mathbb{N}$ often notationally suppressed in what follows, let

$$(4) \quad P_\vartheta := M_{n, \mu(\vartheta)} \quad \text{for } \vartheta \in \Theta_d$$

DEFINITION 1.1. *Let $d, n \in \mathbb{N}$. The (full) latent class model for a sample of size n of combined results of d diagnostic tests with unknown characteristics and for a state with unknown prevalence is $\mathcal{P}_d := (P_\vartheta : \vartheta \in \Theta_d)$.*

The interpretation of the parameter $\vartheta = (\pi, \chi)$ in this model is as follows: π_1 is the prevalence of positive states and χ is the joint characteristics of the d diagnostic tests.

For example, let $d = 2$. Then $\chi_{01|0}$ is the probability that a random negative (see the last bit of the subscript) is diagnosed negative by the first test (see the first bit of the subscript) and positive by the second (see the second bit of the subscript). And $\chi_{0+|0} = \chi_{00|0} + \chi_{01|0}$ is then accordingly the probability that a random negative is diagnosed negative by the first test, that is, the specificity of the first test. More systematically, and introducing a notation used below, we put

$$(5) \quad \chi_{\iota|i}^{(1)} := \chi_{\iota+|i} \quad \text{and} \quad \chi_{\iota|i}^{(2)} := \chi_{+|\iota i} \quad \text{for } i, \iota \in \{0, 1\}$$

and regard $\chi^{(1)}, \chi^{(2)} \in \text{mark}(\{0, 1\}, \{0, 1\})$ as the characteristics of the first and of the second test, respectively.

Coming back to general d , formula (2) gives the joint density of a true state determination together with the results of the d tests, for an item picked at random from the whole population, and $\mu(\vartheta)$ is the marginal density corresponding to unobservability of the true state. Finally, the multinomial distribution $P_\vartheta = M_{n, \mu(\vartheta)}$ models testing thus a random sample of size n from

the (conceptually infinite) population, and counting just the number of occurrences of each possible combination of the d test results.

In this paper, motivated by the application sketched in Subsection 1.5 below, we are mainly interested in the case of $d = 2$, and here in particular in the submodel assuming that the specificity of the first test is at most equal to the specificity of the second. In terms of the parameter $\vartheta = (\pi, \chi) \in \Theta_2$ and with the notation introduced in (5) above, this assumption is expressed as $\chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)}$.

DEFINITION 1.2. *Let $n \in \mathbb{N}$. In this paper, the restricted latent class model for a sample of size n of combined results of two diagnostic tests with unknown characteristics and for a state with unknown prevalence is $\mathcal{P}_{2,\leq} := (P_\vartheta : \vartheta \in \Theta_{2,\leq})$ with $\Theta_{2,\leq} := \{(\pi, \chi) \in \Theta_2 : \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)}\}$.*

1.5. Example: A comparison of two tests for diagnosing toxigenic *Clostridium difficile*. *Clostridium difficile* is a certain species of bacteria. Some of these, called *toxigenic*, have the potential to produce one or both of certain toxins, called *A* and *B*. Toxigenic *Clostridium difficile* is responsible for one of the most prevalent infections of the human gut. It may lead to severe courses of infection and is easily transmitted in hospitals. A fast and accurate diagnosis would be highly desirable for initiating adequate therapy and preventing transmissions to other patients. Unfortunately, so far no diagnostic test, not even a complex and time-consuming one, has been proven to be highly accurate, that is, with specificity and sensitivity close to 1.

Available diagnostic tests are applied to stool specimens of patients with diarrhoea, using one of the following three methods, with details to be specified. The first, simple and a matter of a few hours, consists in performing an enzyme-immuno-assay (*EIA*) for the direct detection of toxin A or B in the stool specimen. The second, taking about 3 days, consists in trying to culture *Clostridium difficile* (possibly nontoxigenic) from the stool specimen on an appropriate medium and applying then a “confirmatory test” for toxin A or B, for example an *EIA* as above, to any cultured colonies. The third, again taking about 3 days, tests the cytotoxic potential of the stool specimen by applying it to a vero-cell culture (*cytotoxicity neutralisation test*). For several such tests, different accuracy values were published during the last years, often obtained by assuming the cytotoxicity neutralisation test to be a sufficiently accurate reference test or “gold standard”, see [6, 7] for appropriate references.

One goal of [6, 7] was to compare a test according to the first method described above (*Test 1* or *direct test*) with a test according to the second method, with the confirmatory test being the same *EIA* as in the direct test

(*Test 2 or culture test*). Both tests were applied to each stool specimen of a sample of size 256, consisting of all liquid specimens sent to a microbiological laboratory during two consecutive months. The observed data were

$$(6) \quad \begin{array}{ccc|cc} k_{00} = 210 & k_{01} = 20 & k_{0+} = 230 \\ k_{10} = 4 & k_{11} = 22 & k_{1+} = 26 \\ \hline k_{++} = 214 & k_{+1} = 42 & k_{++} = 256 \end{array}$$

where, for example, k_{01} is the number of specimens tested negative with Test 1 and positive with Test 2. True states were unobservable. The prevalence of toxigenic Clostridium difficile, in the population of all liquid stool samples sent to a laboratory for microbiological investigation, is certainly not known precisely, but is believed to be very roughly 15%. So far it seems natural to use the full latent class model \mathcal{P}_2 for analyzing the data. However, as the EIA is applied in Test 1 to the whole stool specimen and in Test 2 only to a part of a culture from the specimen already identified as Clostridium difficile, it seems very plausible to assume that Test 2 is at least as specific as Test 1. This suggests that the restricted latent class model $\mathcal{P}_{2,\leq}$ could be used, and that then the superiority of Test 2 would follow if the latter can be proved to be also more sensitive than Test 1. Theorem 1.1 in the next section is formulated with a view towards situations like the present, taking into account both models, \mathcal{P}_2 and $\mathcal{P}_{2,\leq}$.

1.6. Main results. Application to the comparison of tests for diagnosing toxigenic Clostridium difficile.

THEOREM 1.1. *Let $\beta \in [0, 1]$, $n \in \mathbb{N}$,*

$$(7) \quad \Delta : \left\{ k \in \mathbb{N}_0^{\{0,1\}^2} : k_{++} = n \right\} \rightarrow [-1, 1]$$

be a function, and $\mathcal{M} := (\mathbf{M}_{n,q} : q \in \text{prob}(\{0, 1\}^2))$ be a quadrinomial model.

A. *The following three assertions are equivalent:*

(i) Δ is a lower β -confidence bound in the model \mathcal{M} and for the parameter

$$(8) \quad q \mapsto q_{01} - q_{10}$$

(ii) Δ is a lower β -confidence bound in the full latent class model \mathcal{P}_2 and for the parameter

$$(9) \quad (\pi, \chi) \mapsto \pi_1 \left(\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} \right) - (1 - \pi_1) \left(\chi_{0|0}^{(2)} - \chi_{0|0}^{(1)} \right)$$

(iii) Δ is a lower β -confidence bound in the restricted latent class model $\mathcal{P}_{2,\leq}$ and for the parameter

$$(10) \quad (\pi, \chi) \mapsto \pi_1 \left(\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} \right)$$

B. Let $\underline{\Delta}$ obey the above conditions (i)-(iii) and let Δ be another such function. Then Δ is worse than $\underline{\Delta}$ as a lower β -confidence bound for $(\mathcal{M}, (8))$ iff it is so for $(\mathcal{P}_2, (9))$, and if it is so for $(\mathcal{P}_{2,\leq}, (10))$. (Once “iff”, once “if”.)

C. If $\underline{\Delta}$ is admissible as a β -confidence bound for one of the problems $(\mathcal{M}, (8))$ and $(\mathcal{P}_2, (9))$, then so it is for the other and for $(\mathcal{P}_{2,\leq}, (10))$.

See Section 4 for a proof of this and the other two theorems of this subsection. We proceed to illustrate Theorem 1.1 by its application to the example from Subsection 1.5. Let $\beta \in [0, 1]$ and $n \in \mathbb{N}$ be fixed. Wanted is a “good” confidence bound $\underline{\Delta}$ as in (7) and (iii) above. Parts B and C Theorem 1.1 suggest choosing $\underline{\Delta}$ to be a “good” confidence bound as in (i). We put

$$\underline{\Delta}(k) := \ell(k_{01}, k_{10}, k_{00} + k_{11}) \quad \text{for } k \in \mathbb{N}_0^{\{0,1\}^2} \text{ with } k_{++} = n$$

where $\ell : \{k \in \mathbb{N}_0^3 : k_+ = n\} \rightarrow [-1, 1]$ is the Lloyd-Moldovan lower β -confidence bound for the coordinate difference $\text{prob}(\{1, 2, 3\}) \ni p \mapsto p_1 - p_2$ in the trinomial model $(M_{n,p} : p \in \text{prob}(\{1, 2, 3\}))$, see Subsection 1.7. Then $\underline{\Delta}$ satisfies (7) and (i). With $\beta = 0.95$ and the data k from (6), we get

$$\underline{\Delta}(k) = \ell(20, 4, 232) = 0.0320$$

as our lower confidence bound in (i), corresponding to the point estimate $\frac{20}{256} - \frac{4}{256} = \frac{1}{16} = 0.0625$. (Here and below, numbers in typescript like 0.0320 are rounded consistently with the inequalities claimed.) Thus, assuming the restricted latent class model $\mathcal{P}_{2,\leq}$ and using (iii), we get the confidence statement

$$(11) \quad \chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} \geq \frac{0.0320}{\pi_1}$$

with $\pi_1 > 0$, so that Test 2 is significantly more sensitive than Test 1 and hence, being at least as specific by assumption, significantly better. Without any upper bound on the prevalence π_1 , the best lower bound for the sensitivity gain $\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)}$ of the culture test with respect to the direct test we can obtain from (11) is 0.0320. But assuming some plausible upper bound implies a dramatic sensitivity gain; for example, $\pi_1 \leq 0.15$ yields $\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} \geq 0.0320/0.15 = 0.21$. This would imply in particular $\chi_{1|1}^{(1)} \leq 1 - (\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)}) \leq 1 - 0.21 = 0.79$ and hence a very poor sensitivity of the direct test. It is remarkable that the latter conclusion, with a slightly larger bound, can be obtained without any assumption on the prevalence by using the following theorems, see (17) and (19) below.

THEOREM 1.2. Let $\beta \in [0, 1]$, $n \in \mathbb{N}$,

$$(12) \quad \bar{S} : \left\{ k \in \mathbb{N}_0^{\{0,1\}^2} : k_{++} = n \right\} \rightarrow [0, 1]$$

be a function, and $\mathcal{M} := (\mathbf{M}_{n,q} : q \in \text{prob}(\{0, 1\}^2))$ be a quadrinomial model.

A. \bar{S} is an upper β -confidence bound in the model \mathcal{M} and for the parameter

$$(13) \quad q \mapsto \frac{q_{1+}}{q_{1+} + q_{01}} \vee \left(\frac{q_{11}}{(q_{1+} - q_{10})^+} \wedge 1 \right) \quad \text{with} \quad \frac{0}{0} := 1$$

iff it is so in the restricted latent class model $\mathcal{P}_{2,\leq}$ and for the parameter

$$(14) \quad (\pi, \chi) \mapsto \chi_{1|1}^{(2)}$$

B. Let \bar{S} obey the equivalent conditions from part A, and let \tilde{S} be another such function. If \tilde{S} is worse than \bar{S} as an upper β -confidence bound for $(\mathcal{P}_{2,\leq}, (14))$, then so it is for $(\mathcal{M}, (13))$.

C. If \bar{S} is admissible as a β -confidence bound for $(\mathcal{M}, (13))$, then so it is for $(\mathcal{P}_{2,\leq}, (14))$.

We get a confidence bound for $(\mathcal{M}, (13))$, as needed for applying Theorem 1.2 A, from confidence bounds in certain trinomial models, similarly to but slightly less obviously than for the situation of Theorem 1.1:

THEOREM 1.3. Let $\beta \in [0, 1]$, $n \in \mathbb{N}$, and $u : \{k \in \mathbb{N}_0^3 : k_+ \leq n\} \rightarrow [0, \infty]$ be a function such that, for every $m \in \{0, \dots, n\}$, the restriction of u to $\{k \in \mathbb{N}_0^3 : k_+ = m\}$ is an upper β -confidence bound in the trinomial model $(\mathbf{M}_{m,p} : p \in \text{prob}(\{1, 2, 3\}))$ and for the parameter

$$(15) \quad p \mapsto (1 - p_2) \vee \left(\frac{1 - p_1 - p_2}{(1 - 2p_1)^+} \wedge 1 \right) \quad \text{with} \quad \frac{0}{0} := 1$$

Then the function

$$(16) \quad \left\{ k \in \mathbb{N}_0^{\{0,1\}^2} : k_{++} = n \right\} \ni k \mapsto u(k_{10}, k_{01}, k_{11})$$

is an upper β -confidence bound for $(\mathcal{P}_{2,\leq}, (14))$.

As we are not aware of a function u as assumed in Theorem 1.3 and also well-founded and easily available for practical computation, we use here

the following ad hoc method: Let u_0 denote the Lloyd-Moldovan upper β -confidence bound corresponding to the lower bound ℓ used above. Then, since

$$\begin{aligned} \text{R.H.S.(15)} &= (1 - p_2) \vee \left(\frac{1 - 2p_1 + p_1 - p_2}{(1 - 2p_1)^+} \wedge 1 \right) \quad \text{with} \quad \frac{0}{0} := 1 \\ &\leq (1 + p_1 - p_2) \wedge 1 \end{aligned}$$

for $p \in \text{prob}(\{1, 2, 3\})$, we may take $u := (1 + u_0) \wedge 1$ in Theorem 1.3. Applied to our data (6), this yields $u(k_{10}, k_{01}, k_{11}) = (1 + u_0(4, 20, 22)) \wedge 1 = 0.83$ and thus

$$(17) \quad \chi_{1|1}^{(1)} \leq 0.83$$

with confidence 0.95, in the restricted latent class model without further assumptions.

Going back to (11), obtained under the restricted latent class model, Part A of Theorem 1.1 suggests that we should perhaps rather state

$$(18) \quad \chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} \geq \frac{0.0320}{\pi_1} + \frac{1 - \pi_1}{\pi_1} (\chi_{0|0}^{(2)} - \chi_{0|0}^{(1)})$$

as a valid confidence statement under the full latent class model. This not only makes obvious the effect of the possibility $\chi_{0|0}^{(2)} - \chi_{0|0}^{(1)} < 0$ in the larger model, drastically decreasing the lower bound for the sensitivity difference, but also the possibly drastic increase if we actually have $\chi_{0|0}^{(2)} - \chi_{0|0}^{(1)} > 0$ and π_1 rather small.

So far, we have for simplicity only considered part of the data from [6, 7]. There, we actually applied the direct test and three versions of the culture test, differing in the culture media used, to each of the 256 specimens. The media are called I, II, III in [6, 7], and here (6) presents just the results for the direct test and for the culture test with medium II. Bounds analogous to the above lower confidence bound for the sensitivity gain through culturing with medium II, with the exemplary assumption $\pi_1 \leq 0.15$, were computed for media I and III, resulting in -0.04 for I (so no statistically significant gain here) and 0.02 for III. For obtaining the upper confidence bound on the sensitivity of the direct test, without any assumption on the prevalence, we compared in [7] the direct test with the logical oring of the three culture tests, which diagnoses a specimen as positive if at least one of the three does so, yielding the data $k_{00} = 209$, $k_{01} = 21$, $k_{10} = 4$, $k_{11} = 22$ rather than (6), and hence the confidence statement

$$(19) \quad \chi_{1|1}^{(1)} \leq (1 + u_0(4, 21, 22)) \wedge 1 = 0.81$$

1.7. The Lloyd-Moldovan confidence bound for a coordinate difference of a multinomial parameter. The best currently available confidence bound ℓ as needed in Theorem 1.1 appears to be the one proposed and implemented by Lloyd and Moldovan [5]: To compute it, load their program into R with `load("sm_file_SIM2708_2")`, type `bcl(c1.side=-1)`, where “-1” asks for the lower rather than the default upper bound obtainable with just `bcl()`, enter the three numbers $x = k_1$, $t = k_1 + k_2$ und $n = k_1 + k_2 + k_3$, with return after each, and then a few more returns, assuming here $\beta = 0.95$ for simplicity.

1.8. Example: Robust upper confidence bounds for the sensitivities of diagnostic tests for coronary artery disease. This subsection uses part of a standard dataset, given in [4, Table 5] and [8, pp. 8, 17, 22] and drawn from [10], to exemplify the final sentence of Subsection 1.1. We consider evaluating two diagnostic tests for coronary artery disease (*CAD*). This disease is the most frequent cause of myocardic infarction, which in turn is the most frequent cause of death in developed countries.

The first test considered is a dichotomized exercise stress test (*EST*), the second a dichotomized chest pain history (*CPH*). These two tests and a dichotomized arteriography (*A*) were performed on each of 1465 men. The dataset is a three-way table of counts $k \in \mathbb{N}_0^{\{0,1\}^3}$ with $k_{+++} = 1465$ and with the indexing here corresponding to the ordering *EST*, *CPH*, *A*: $k_{000} = 151$ men negative for all three tests, $k_{001} = 25$ positive only for *A*, $k_{010} = 176$ positive only for *CPH*, $k_{011} = 183$, $k_{100} = 46$ positive only for *EST*, $k_{101} = 29$, $k_{110} = 69$, $k_{111} = 786$. As usual, it is assumed that the 1465 trivariate observables are independent and identically distributed. Let $k^{\text{EST}} := (k_{i+j} : (i, j) \in \{0, 1\}^2)$ denote the marginal table for just the results of *EST* and *A*, and let analogously $k^{\text{CPH}} := (k_{i+j} : (i, j) \in \{0, 1\}^2)$ be the marginal table for *CPH* and *A*. Thus

$$\begin{array}{llll} k_{00}^{\text{EST}} = 327 & k_{01}^{\text{EST}} = 208 & k_{00}^{\text{CPH}} = 197 & k_{01}^{\text{CPH}} = 54 \\ k_{10}^{\text{EST}} = 115 & k_{11}^{\text{EST}} = 815 & k_{10}^{\text{CPH}} = 245 & k_{11}^{\text{CPH}} = 969 \end{array}$$

If, as in [4, 8], the test *A* is assumed to be perfect, then we get the following four separate 95% binomial confidence statements (ignoring corrections for quadruplicity) for the sensitivities Se^{EST} and Se^{CPH} and the specificities Sp^{EST} and Sp^{CPH} of the tests *EST* and *CPH*,

$$(20) \quad \begin{array}{lll} 0.770 \leq \text{Se}^{\text{EST}} \leq 0.821 & 0.931 \leq \text{Se}^{\text{CPH}} \leq 0.961 \\ 0.696 \leq \text{Sp}^{\text{EST}} \leq 0.781 & 0.398 \leq \text{Sp}^{\text{CPH}} \leq 0.494 \end{array}$$

using, for example, the R-command `binom.test(c(815,208))` for the first interval, and we may conclude that neither *EST* nor *CPH* is sufficiently ac-

curate. The perfectness of A means that its specificity Sp^A and its sensitivity Se^A are both equal to 1, or rather practically very nearly so. Here the assumption $Sp^A = 1$ appears quite reasonable from the medical point of view, but $Se^A = 1$ does not. Using now only the weaker assumption $Sp^{EST} \leq Sp^A$ or $Sp^{CPH} \leq Sp^A$, respectively, we get the two separate 95% upper confidence bound statements

$$Se^{EST} \leq 0.945 \quad Se^{CPH} \leq 1$$

using Theorem 1.3 as in Subsection 1.6, computing $u(115, 208, 815)$ and $u(245, 54, 969)$ with the ad hoc function u indicated there. The second bound is unfortunately trivial, but the first, while of course weaker than the statement from (20) obtained under a much stronger assumption, is still good enough to show that EST is far from perfect: EST fails to diagnose CAD for at least every twentieth CAD patient.

2. Auxiliary results on latent class models. In this section we describe images, under various parameters of interest, of the preimage $\mu^{-1}(\{q\}) = \{\vartheta = (\pi, \chi) \in \Theta_d : \mu(\vartheta) = q\}$ in Subsections 2.1 and 2.2, and of a similar preimage with $\Theta_{2,\leq}$ in place of Θ_d in Subsection 2.3, of a given $q \in \text{prob}(\{0, 1\}^d)$ under the function μ defined in (3). Informally speaking, this amounts to determining the exact joint range of the possible values of the prevalence, sensitivities, and specificities (Lemma 2.1 for $d = 1$ and Lemma 2.3 for $d = 2$), or certain functions of these (Lemmas 2.4-2.16), assuming the density q of the joint test results as known or, in a more practical interpretation, estimated with high accuracy from a very large sample of joint test results. For example, using here, for the purpose of illustration only, $q = \hat{q} := \frac{k}{k_{++}}$ based on the data k from (6), that is

$$\begin{array}{lll|l} \hat{q}_{00} = 0.820 & \hat{q}_{01} = 0.078 & \hat{q}_{0+} = 0.90 \\ \hat{q}_{10} = 0.016 & \hat{q}_{11} = 0.083 & \hat{q}_{1+} = 0.10 \\ \hline \hat{q}_{+0} = 0.84 & \hat{q}_{+1} = 0.16 & \hat{q}_{++} = 1 \end{array}$$

the pictures of C and C_{\leq} displayed below near the corresponding Lemmas 2.5 and 2.10 show as hatched regions the exact joint ranges of the possible values of the prevalence and the sensitivity difference, the first in the full latent class model, and the second in the restricted one.

All these lemmas, needed to prove Theorems 1.1 and 1.3 in Section 4 below, are proved in Section 3, where the less interesting results of Subsections 2.1 and 2.2 are used for obtaining the more important results of Subsection 2.3.

We have found it suggestive to denote below certain “variables” with Pr , Sp , Se , Sp_1 , Sp_2 , Se_1 , Se_2 , and ΔSe . Perhaps it should be pointed out that,

for example, denoting a variable by Se_1 in Lemma 2.6 does not imply that Se_1 be the first coordinate of some tuple called Se . This differs from our use of subscripts for π and χ , for example in the definition of A in Lemma 2.3, where π_1 is understood to be the last coordinate of $\pi = (\pi_0, \pi_1)$.

2.1. *The case $d = 1$ and a partial reduction to it.* In this subsection, we write more precisely μ_d for the function μ from (3).

LEMMA 2.1. *If $q \in \text{prob}(\{0, 1\})$, then $\{(\pi_1, \chi_{0|0}, \chi_{1|1}) : (\pi, \chi) \in \mu_1^{-1}(\{q\})\} = \{(\text{Pr}, \text{Sp}, \text{Se}) \in [0, 1]^3 : (1 - \text{Pr})(1 - \text{Sp}) + \text{Pr Se} = q_1\}$.*

We recall the dot notation for functions explained in Subsection 1.2.

LEMMA 2.2. *Let $q \in \text{prob}(\{0, 1\}^2)$. Then*

$$(21) \quad \{(\pi, \chi^{(1)}) : (\pi, \chi) \in \mu_2^{-1}(\{q\})\} = \mu_1^{-1}(\{q_{+}\})$$

$$(22) \quad \{(\pi, \chi^{(2)}) : (\pi, \chi) \in \mu_2^{-1}(\{q\})\} = \mu_1^{-1}(\{q_{+}\})$$

2.2. *The case $d = 2$ for the full latent class model.* In this subsection and in the next one, we return to the shorter notation μ instead of μ_2 , and we assume that $q \in \text{prob}(\{0, 1\}^2)$ is fixed.

LEMMA 2.3. *$A := \{(\pi_1, \chi_{0|0}^{(1)}, \chi_{1|1}^{(1)}, \chi_{0|0}^{(2)}, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\}$ is the nonempty set of all $(\text{Pr}, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in [0, 1]^5$ satisfying the relations*

$$(23) \quad (1 - \text{Pr})(1 - \text{Sp}_1) + \text{Pr Se}_1 = q_{1+}$$

$$(24) \quad (1 - \text{Pr})(1 - \text{Sp}_2) + \text{Pr Se}_2 = q_{+1}$$

$$(25) \quad (1 - \text{Pr})\text{Sp}_1 \wedge \text{Sp}_2 + \text{Pr}(1 - \text{Se}_1 \vee \text{Se}_2) \geq q_{00}$$

$$(26) \quad (1 - \text{Pr})(\text{Sp}_1 + \text{Sp}_2 - 1)^+ + \text{Pr}(1 - \text{Se}_1 - \text{Se}_2)^+ \leq q_{00}$$

or, equivalently,

$$(27) \quad \text{Pr}(\text{Se}_2 - \text{Se}_1) = (1 - \text{Pr})(\text{Sp}_2 - \text{Sp}_1) + q_{01} - q_{10}$$

$$(28) \quad \text{Pr}(\text{Se}_1 + \text{Se}_2 - 1) = (1 - \text{Pr})(\text{Sp}_1 + \text{Sp}_2 - 1) + q_{11} - q_{00}$$

$$(29) \quad -q_{10} \leq \text{Pr}(\text{Se}_2 - \text{Se}_1) \leq q_{01}$$

$$(30) \quad -q_{00} \leq \text{Pr}(\text{Se}_1 + \text{Se}_2 - 1) \leq q_{11}$$

LEMMA 2.4. *$B := \{(\pi_1, \chi_{1|1}^{(1)}, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\}$ is the nonempty set of all $(\text{Pr}, \text{Se}_1, \text{Se}_2) \in [0, 1]^3$ satisfying the relations (29), (30) and*

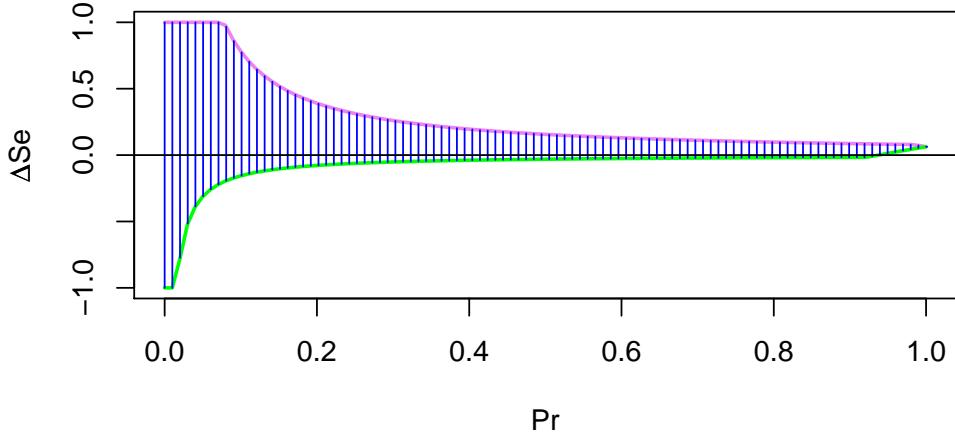
$$(31) \quad \text{Pr} - q_{0+} \leq \text{Pr Se}_1 \leq q_{1+}$$

$$(32) \quad \text{Pr} - q_{+0} \leq \text{Pr Se}_2 \leq q_{+1}$$

LEMMA 2.5. $C := \{(\pi_1, \chi_{1|1}^{(2)} - \chi_{1|1}^{(1)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\}$ is the nonempty set of all $(\Pr, \Delta Se) \in [0, 1] \times [-1, 1]$ satisfying the inequalities

$$(33) \quad \begin{aligned} (-q_{10}) \vee (q_{01} - q_{10} + \Pr - 1) &\leq \Pr \Delta Se \\ &\leq q_{01} \wedge (q_{01} - q_{10} + 1 - \Pr) \end{aligned}$$

C : Full range for Pr and ΔSe , with $q = \hat{q}$



LEMMA 2.6. $D := \{(\pi_1, \chi_{1|1}^{(1)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\}$ is the nonempty set of all $(\Pr, Se_1) \in [0, 1]^2$ satisfying (31).

LEMMA 2.7. $E := \{(\pi_1, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\}$ is the nonempty set of all $(\Pr, Se_2) \in [0, 1]^2$ satisfying (32).

LEMMA 2.8.

$$\begin{aligned} F &:= \{(\chi_{1|1}^{(2)} - \chi_{1|1}^{(1)}) : (\pi, \chi) \in \mu^{-1}(\{q\})\} = [-1, 1] \\ G &:= \{\chi_{1|1}^{(1)} : (\pi, \chi) \in \mu^{-1}(\{q\})\} = [0, 1] \\ H &:= \{\chi_{1|1}^{(2)} : (\pi, \chi) \in \mu^{-1}(\{q\})\} = [0, 1] \\ I &:= \{\pi_1 : (\pi, \chi) \in \mu^{-1}(\{q\})\} = [0, 1] \end{aligned}$$

2.3. *The case $d = 2$ for the restricted latent class model.* We recall that μ denotes μ_2 and that $q \in \text{prob}(\{0, 1\}^2)$ is fixed also in this subsection. Here we describe images A_{\leq} to I_{\leq} analogous to A to I , with $\{\vartheta \in \Theta_{2,\leq} : \mu(\vartheta) = q\}$ in place of $\{\vartheta \in \Theta_2 : \mu(\vartheta) = q\}$. We recall from Definition 1.2 that the subscript

\leq " indicates that the specificity of the first test is assumed to be at most equal to that of the second. Trivially,

$$A_{\leq} := \left\{ (\pi_1, \chi_{0|0}^{(1)}, \chi_{1|1}^{(1)}, \chi_{0|0}^{(2)}, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \right\}$$

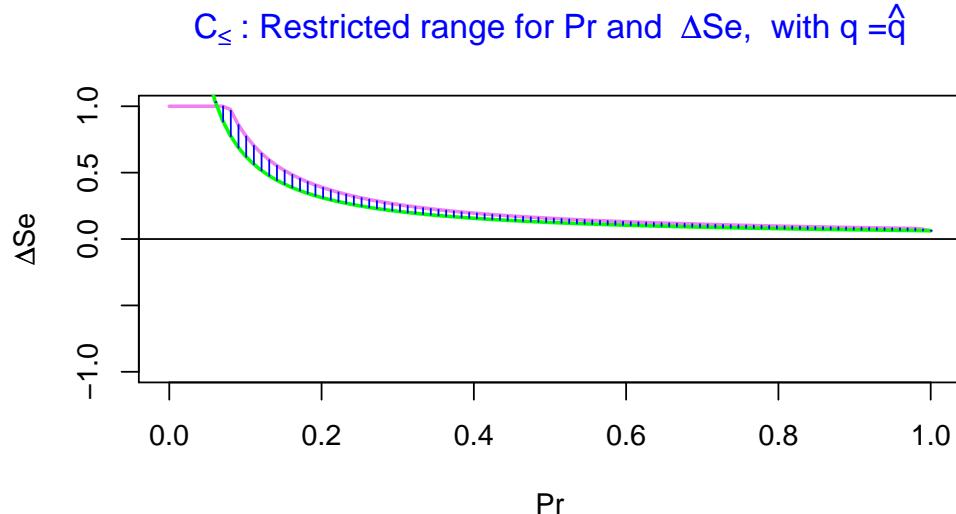
is just the set of all $(\Pr, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in A$ satisfying $\text{Sp}_1 \leq \text{Sp}_2$, and the nonemptiness of this set is proved at the beginning of Section 3 below.

LEMMA 2.9. $B_{\leq} := \left\{ (\pi_1, \chi_{1|1}^{(1)}, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \right\}$ is the nonempty set of all $(\Pr, \text{Se}_1, \text{Se}_2) \in [0, 1]^3$ satisfying the relations (30), (31), (32), and

$$(34) \quad q_{01} - q_{10} \leq \Pr(\text{Se}_2 - \text{Se}_1) \leq q_{01}$$

LEMMA 2.10. $C_{\leq} := \left\{ (\pi_1, \chi_{1|1}^{(2)} - \chi_{1|1}^{(1)}) : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \right\}$ is the nonempty set of all $(\Pr, \Delta\text{Se}) \in [0, 1] \times [-1, 1]$ satisfying the inequalities

$$(35) \quad q_{01} - q_{10} \leq \Pr \Delta\text{Se} \leq q_{01} \wedge (q_{01} - q_{10} + 1 - \Pr)$$



LEMMA 2.11. $D_{\leq} := \left\{ (\pi_1, \chi_{1|1}^{(1)}) : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \right\}$ is the nonempty set of all $(\Pr, \text{Se}_1) \in [0, 1]^2$ satisfying the inequalities

$$(36) \quad \Pr - q_{0+} \leq \Pr \text{Se}_1 \leq q_{1+} \wedge \frac{\Pr + q_{1+} - q_{01}}{2} \wedge (\Pr + q_{10} - q_{01})$$

LEMMA 2.12. $E_{\leq} := \{ (\pi_1, \chi_{1|1}^{(2)}) : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \}$ is the nonempty set of all $(\text{Pr}, \text{Se}_2) \in [0, 1]^2$ satisfying the inequalities

$$(37) \quad (\text{Pr} - q_{+0}) \vee \frac{\text{Pr} + q_{01} - q_{+0}}{2} \vee (q_{01} - q_{10}) \leq \text{Pr Se}_2 \leq q_{+1}$$

LEMMA 2.13. $F_{\leq} := \{ \chi_{1|1}^{(2)} - \chi_{1|1}^{(1)} : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \}$ is the nonempty interval $[q_{01} - q_{10}, 1]$ if $q_{01} - q_{10} > 0$, and $[-1, 1]$ if $q_{01} - q_{10} \leq 0$.

LEMMA 2.14. $G_{\leq} := \{ \chi_{1|1}^{(1)} : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \}$ is the nonempty interval

$$\left[0, \frac{q_{1+}}{q_{1+} + q_{01}} \vee \left(\frac{q_{11}}{(q_{+1} - q_{10})^+} \wedge 1 \right) \right] \quad \text{with} \quad \frac{0}{0} := 1$$

LEMMA 2.15. $H_{\leq} := \{ \chi_{1|1}^{(2)} : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \}$ is the nonempty interval

$$\left[\frac{q_{01}}{q_{0+} + q_{10}} \wedge \frac{(q_{01} - q_{10})^+}{q_{0+} - q_{10}}, 1 \right] \quad \text{with} \quad \frac{0}{0} := 1$$

LEMMA 2.16. $I_{\leq} := \{ \pi_1 : (\pi, \chi) \in \mu^{-1}(\{q\}), \chi_{0|0}^{(1)} \leq \chi_{0|0}^{(2)} \}$ is the nonempty interval

$$\left[(q_{01} - q_{10})^+, (1 - (q_{10} - q_{01})^+) \vee (q_{10} - q_{01}) \right]$$

3. Proofs for Section 2. Let us first address the nonemptiness of the sets A to I_{\leq} . Below, we prove Lemmas 2.3-2.16 ignoring the word “nonempty”. So, strictly speaking, we should rather write something like “Proof of Weak Lemma 2.3” and so on below. We next observe that, say, the interval then known to equal G_{\leq} by Lemma 2.14 is nonempty, as it contains zero. Hence A_{\leq} is nonempty, since G_{\leq} is the image of A_{\leq} under some function. Hence $A \supseteq A_{\leq}$ is nonempty. Hence the remaining sets are nonempty, as they are images of A or A_{\leq} under certain functions.

PROOF OF LEMMA 2.1. If $(\pi, \chi) \in \mu_1^{-1}(\{q\})$, then we have in particular $(\pi_1, \chi_{0|0}, \chi_{1|1}) \in [0, 1]^3$ and $(1 - \pi_1)(1 - \chi_{0|0}) + \pi_1 \chi_{1|1} = (\mu_1(\pi, \chi))_1 = q_1$. This shows that “ \subseteq ” holds in the claimed equality. If, conversely, $(\text{Pr}, \text{Sp}, \text{Se})$ belongs to the second set, and if we put $\pi_0 := 1 - \text{Pr}$, $\pi_1 := \text{Pr}$, $\chi_{0|0} := \text{Sp}$, $\chi_{1|0} := 1 - \text{Sp}$, $\chi_{0|1} := 1 - \text{Se}$, $\chi_{1|1} := \text{Se}$, then $(\pi, \chi) \in \mu_1^{-1}(\{q\})$. Thus “ \supseteq ” holds as well. \square

PROOF OF LEMMA 2.2. If $(\pi, \chi) \in \mu_2^{-1}(\{q\})$, then $(\pi, \chi^{(1)}) \in \Theta_1$ and for $\iota \in \{0, 1\}$ we have

$$\mu_1(\pi, \chi^{(1)}) = \sum_{i=0}^1 \pi_i \chi_{\iota|i}^{(1)} = \sum_{i=0}^1 \sum_{\kappa=0}^1 \pi_i \chi_{\iota\kappa|i} = \sum_{\kappa=0}^1 q_{\iota\kappa} = q_{\iota+}$$

This proves “ \subseteq ” in (21). If $(\pi, \psi) \in \mu_1^{-1}(\{q_{\cdot+}\})$, then, by

$$\chi_{j|i} := \frac{q_j}{q_{j_1+}} \psi_{j_1|i} \quad \text{for } (i, j) \in \{0, 1\} \times \{0, 1\}^2$$

with the nonstandard convention $\frac{0}{0} := \frac{1}{2}$, we define a $\chi \in \text{mark}(\{0, 1\}, \{0, 1\}^2)$ with $\chi^{(1)} = \psi$ and

$$(\mu_2(\pi, \chi))_j = \sum_{i=0}^1 \pi_i \chi_{j|i} = \frac{q_j}{q_{j_1+}} \sum_{i=0}^1 \pi_i \psi_{j_1|i} = q_j \quad \text{for } j \in \{0, 1\}^2$$

This proves “ \supseteq ” in (21). The proof of (22) is analogous. \square

PROOF OF LEMMA 2.3. Call A' the set claimed to equal A up to line (26). If $\vartheta = (\pi, \chi) \in \Theta_2$, then obviously

$$(38) \quad (\pi_1, \chi_{0+|0}, \chi_{1+|1}, \chi_{+0|0}, \chi_{+1|1}) \in [0, 1]^5$$

and, using (3) and identities like $\pi_0 = 1 - \pi_1$ and $\chi_{1+|0} = 1 - \chi_{0+|0}$, the condition $\mu(\vartheta) = q$ is seen to be equivalent to the system of three equations

$$(39) \quad (1 - \pi_1)(1 - \chi_{0+|0}) + \pi_1 \chi_{1+|1} = q_{1+}$$

$$(40) \quad (1 - \pi_1)(1 - \chi_{+0|0}) + \pi_1 \chi_{+1|1} = q_{+1}$$

$$(41) \quad (1 - \pi_1)\chi_{00|0} + \pi_1 \chi_{00|1} = q_{00}$$

Using first $\chi_{00|0} \leq \chi_{0+|0} \wedge \chi_{+0|0}$ and $\chi_{00|1} \leq \chi_{0+|1} \wedge \chi_{+0|1} = (1 - \chi_{1+|1}) \wedge (1 - \chi_{+1|1})$ and second $\chi_{00|0} = \chi_{0+|0} + \chi_{+0|0} - (1 - \chi_{11|0}) \geq (\chi_{0+|0} + \chi_{+0|0} - 1)^+$ and $\chi_{00|1} = 1 + \chi_{11|1} - \chi_{1+|1} - \chi_{+1|1} \geq (1 - \chi_{1+|1} - \chi_{+1|1})^+$, we see that equation (41) would imply the two inequalities

$$\begin{aligned} (1 - \pi_1)\chi_{0+|0} \wedge \chi_{+0|0} + \pi_1(1 - \chi_{1+|1}) \wedge (1 - \chi_{+1|1}) &\geq q_{00} \\ (1 - \pi_1)(\chi_{0+|0} + \chi_{+0|0} - 1)^+ + \pi_1(1 - \chi_{1+|1} - \chi_{+1|1})^+ &\leq q_{00} \end{aligned}$$

Thus for $\vartheta \in \Theta_2$ with $\mu(\vartheta) = q$, the left hand side of (38) belongs to A' . Hence $A \subseteq A'$.

To prove the reversed inclusion, let $(\text{Pr}, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in A'$. Put $\pi = (\pi_0, \pi_1) := (1 - \text{Pr}, \text{Pr})$. Choose two numbers

$$\begin{aligned}\chi_{00|0} &\in [(\text{Sp}_1 + \text{Sp}_2 - 1)^+, \text{Sp}_1 \wedge \text{Sp}_2] \\ \chi_{00|1} &\in [(1 - \text{Se}_1 - \text{Se}_2)^+, (1 - \text{Se}_1) \wedge (1 - \text{Se}_2)]\end{aligned}$$

such that

$$(1 - \text{Pr})\chi_{00|0} + \text{Pr} \chi_{00|1} = q_{00}$$

This is possible by connectedness, since the two intervals above are nonempty and we would get " $\leq q_{00}$ " by choosing the lower endpoints and " $\geq q_{00}$ " for the upper ones. Now put

$$\begin{aligned}\chi_{01|0} &:= \text{Sp}_1 - \chi_{00|0} & \chi_{01|1} &:= 1 - \text{Se}_1 - \chi_{00|1} \\ \chi_{10|0} &:= \text{Sp}_2 - \chi_{00|0} & \chi_{10|1} &:= 1 - \text{Se}_2 - \chi_{00|1} \\ \chi_{11|0} &:= 1 - \text{Sp}_1 - \text{Sp}_2 + \chi_{00|0} & \chi_{11|1} &:= \text{Se}_1 + \text{Se}_2 - 1 + \chi_{00|1}\end{aligned}$$

Then $(\pi, \chi) \in \Theta_2$ satisfies the equations (39)-(41), so that $\mu(\vartheta) = q$, and the corresponding element of A is $(\text{Pr}, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2)$. Hence we also have $A' \subseteq A$.

Obviously, equations (23) and (24) are jointly equivalent to (27) and (28), by addition and subtraction. In the presence of (23) and (24), we have

$$\begin{aligned}(1 - \text{Pr}) \text{Sp}_1 \wedge \text{Sp}_2 &= 1 - \text{Pr} - (1 - \text{Pr})(1 - \text{Sp}_1) \vee (1 - \text{Sp}_2) \\ &= 1 - \text{Pr} - (q_{1+} - \text{Pr} \text{Se}_1) \vee (q_{+1} - \text{Pr} \text{Se}_2)\end{aligned}$$

so that, by inserting and rearranging, inequality (25) is equivalent to

$$\text{Pr} \text{Se}_1 \vee \text{Se}_2 + (q_{10} - \text{Pr} \text{Se}_1) \vee (q_{01} - \text{Pr} \text{Se}_2) \leq q_{01} + q_{10}$$

which, by considering separately the four cases $a \vee b + c \vee d = a + c$ etc., simplifies to (29). Finally, in the presence of (29), inequality (26) is equivalent to $(q_{00} - q_{11} - x)^+ + x^+ \leq q_{00}$ with $x := \text{Pr}(1 - \text{Se}_1 - \text{Se}_2)$, which simplifies to $-q_{11} \leq x \leq q_{00}$, that is, (30). \square

PROOF OF LEMMA 2.4. Call B' the set claimed to equal B . By Lemma 2.3, we have $(\text{Pr}, \text{Se}_1, \text{Se}_2) \in B$ iff there exist Sp_1, Sp_2 with the quintuple $(\text{Pr}, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in [0, 1]^5$ satisfying (23)-(26) or, equivalently, (27)-(30). So in this case, we have in particular (29) and (30), while (23) and (24) together with $\text{Sp}_1, \text{Sp}_2 \in [0, 1]$ yield (31) and (32).

Conversely, if $(\text{Pr}, \text{Se}_1, \text{Se}_2) \in B'$, then by (31) and (32) we can find $\text{Sp}_1, \text{Sp}_2 \in [0, 1]$ satisfying (23) and (24), and hence (27) and (28), and thus $(\text{Pr}, \text{Se}_1, \text{Se}_2) \in B$. \square

PROOF OF LEMMA 2.5. Call C' the set claimed to equal C . By Lemma 2.4, we have $(\Pr, \Delta Se) \in C$ iff there exist Se_1, Se_2 with $(\Pr, Se_1, Se_2) \in [0, 1]^3$ satisfying (29), (30), (31), (32), and $\Delta Se = Se_2 - Se_1$.

Let $(\Pr, \Delta Se) \in C$ and let Se_1, Se_2 be as just stated. Then (31) and (32) yield

$$(42) \quad \Pr \Delta Se = \Pr Se_2 - \Pr Se_1 \leq q_{+1} - (\Pr - q_{0+}) = q_{01} - q_{10} + 1 - \Pr$$

and similarly

$$\Pr \Delta Se \geq \Pr - q_{+0} - q_{1+} = q_{01} - q_{10} + \Pr - 1$$

Together with (29), the above yields (33).

Conversely, let $(\Pr, \Delta Se) \in C'$. If $\Pr = 0$, then we may put $Se_1 := (\Delta Se)^-$ and $Se_2 := (\Delta Se)^+$, and observe that (\Pr, Se_1, Se_2) then satisfies (29), (30), (31), (32), and $\Delta Se = Se_2 - Se_1$.

So assume $\Pr > 0$. By connectedness we can choose

$$\begin{aligned} Se_1 &\in \left[\left(1 - \frac{q_{0+}}{\Pr} \right) \vee 0, \frac{q_{1+}}{\Pr} \wedge 1 \right] =: [a_1, b_1] \\ Se_2 &\in \left[\left(1 - \frac{q_{+0}}{\Pr} \right) \vee 0, \frac{q_{+1}}{\Pr} \wedge 1 \right] =: [a_2, b_2] \end{aligned}$$

in such a way that $Se_2 - Se_1 = \Delta Se$, since the two intervals above are nonempty and since taking $Se_1 = a_1$ and $Se_2 = b_2$ would yield

$$\begin{aligned} \Pr(Se_2 - Se_1) &= q_{+1} \wedge \Pr - (\Pr - q_{0+}) \vee 0 \\ &= \min\{q_{+1} - \Pr + q_{0+}, q_{+1}, q_{0+}, \Pr\} \\ &\geq \min\{q_{01} - q_{10} + 1 - \Pr, q_{01}, \Pr \Delta Se\} \\ &= \Pr \Delta Se \end{aligned}$$

using (33) in the last step, while $Se_1 = b_1$ and $Se_2 = a_2$ would similarly yield

$$\begin{aligned} \Pr(Se_2 - Se_1) &= (\Pr - q_{+0}) \vee 0 - q_{1+} \wedge \Pr \\ &= \max\{\Pr - q_{+0} - q_{1+}, -q_{+0}, -q_{1+}, -\Pr\} \\ &\leq \max\{q_{01} - q_{10} + \Pr - 1, -q_{10}, \Pr \Delta Se\} \\ &= \Pr \Delta Se \end{aligned}$$

using again (33) in the last step. For every choice of Se_1 and Se_2 as above, the triple (\Pr, Se_1, Se_2) obviously satisfies (29), (31), and (32). To get (30) as well, we have to refine our choice: Since the condition $Se_2 - Se_1 = \Delta Se$ is not affected by a same translation of Se_1 and Se_2 , we could choose Se_1 and Se_2

such that $\text{Se}_i = a_i$ for some i , which always yields $\Pr(\text{Se}_1 + \text{Se}_2 - 1) \leq q_{11}$ as in the case of $i = 1$:

$$\begin{aligned}\Pr(\text{Se}_1 + \text{Se}_2 - 1) &\leq (\Pr - q_{0+}) \vee 0 + q_{+1} \wedge \Pr - \Pr \\ &= \max\{-q_{0+} + q_{+1} \wedge \Pr, q_{+1} \wedge \Pr - \Pr\} \\ &\leq \max\{q_{+1} - q_{0+}, 0\} \\ &\leq q_{11}\end{aligned}$$

Alternatively we could choose Se_1 and Se_2 such that $\text{Se}_i = b_i$ for some i , yielding $\Pr(\text{Se}_1 + \text{Se}_2 - 1) \geq -q_{00}$. By connectedness, then, we can choose Se_1 and Se_2 such that (30) holds. Then $(\Pr, \text{Se}_1, \text{Se}_2) \in D$ and we get $(\Pr, \Delta\text{Se}) = (\Pr, \text{Se}_2 - \text{Se}_1) \in C$. \square

PROOF OF LEMMA 2.6. Call D' the set claimed to equal D . Lemma 2.2 yields $D = \{(\pi_1, \chi_{1|1}) : (\pi, \chi) \in \mu_1^{-1}(q_{+1})\}$, which by Lemma 2.1 equals

$$\{(\Pr, \text{Se}_1) \in [0, 1]^2 : \exists \text{Sp}_1 \in [0, 1] \text{ with } (1 - \Pr)(1 - \text{Sp}_1) + \Pr \text{Se}_1 = q_{1+}\}$$

Thus, if $(\Pr, \text{Se}_1) \in D$ and if Sp_1 is chosen according to the above, then using $\text{Sp}_1 \geq 0$ and $\text{Sp}_1 \leq 1$ yields (31) and hence $(\Pr, \text{Se}_1) \in D'$. Conversely, if $(\Pr, \text{Se}_1) \in D'$, then $\text{Sp}_1 := 1 - (q_{1+} - \Pr \text{Se}_1)/(1 - \Pr) \in [0, 1]$, even if $\Pr = 1$ using $0/0 := 0$, hence $(\Pr, \text{Se}_1) \in D$. \square

PROOF OF LEMMA 2.7. As above for Lemma 2.6. \square

PROOF OF LEMMA 2.8. In each case, the “ \subseteq ” claim is trivially true. To prove “ \supseteq ”, use Lemmas 2.5, 2.6, 2.7 with $\Pr = 0$ for F, G, H , and Lemma 2.6 with $\text{Se}_1 = 0$ for I. \square

PROOF OF LEMMA 2.9. Call B'_{\leq} the set claimed to equal B_{\leq} . By Lemma 2.3, we have $(\Pr, \text{Se}_1, \text{Se}_2) \in B_{\leq}$ iff there exist Sp_1, Sp_2 with the quintuple $(\Pr, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in [0, 1]^5$ satisfying (23)-(26), or equivalently (27)-(30), and additionally

$$(43) \quad \text{Sp}_1 \leq \text{Sp}_2$$

Let $(\Pr, \text{Se}_1, \text{Se}_2) \in B_{\leq}$. Then Lemma 2.4 and $B_{\leq} \subseteq B$ yield (29)-(32), and using (27) and (43), we can sharpen (29) to (34), so that $(\Pr, \text{Se}_1, \text{Se}_2) \in B'_{\leq}$.

Conversely, let $(\Pr, \text{Se}_1, \text{Se}_2) \in B'_{\leq}$. Then, since (34) implies (29), Lemma 2.4 yields $(\Pr, \text{Se}_1, \text{Se}_2) \in B$, so that there exist $\text{Sp}_1, \text{Sp}_2 \in [0, 1]$ such that $(\Pr, \text{Sp}_1, \text{Se}_1, \text{Sp}_2, \text{Se}_2) \in A$. If $\Pr = 1$, then by Lemma 2.3 we can choose e.g. $\text{Sp}_1 = \text{Sp}_2 = \frac{1}{2}$, since (27)-(30) remain unaffected, and hence get (43). If $\Pr < 1$, then (27) and the left hand inequality in (34) yield (43). Thus $(\Pr, \text{Se}_1, \text{Se}_2) \in B_{\leq}$. \square

PROOF OF LEMMA 2.10. Call C'_{\leq} the set claimed to equal C_{\leq} . By Lemma 2.9, we have $(Pr, \Delta Se) \in C_{\leq}$ iff there exist Se_1, Se_2 with $(Pr, Se_1, Se_2) \in [0, 1]^3$ satisfying (30), (31), (32), (34), and $\Delta Se = Se_2 - Se_1$.

Let $(Pr, \Delta Se) \in C_{\leq}$ and let Se_1, Se_2 be as just stated. Then (31) and (32) yield (42), and together with (34) this yields (35), hence $(Pr, \Delta Se) \in C'_{\leq}$.

Conversely, let $(Pr, \Delta Se) \in C'_{\leq}$. Then, since (35) implies (33), Lemma 2.5 yields $(Pr, \Delta Se) \in C$, so that there exist Se_1, Se_2 with $(Pr, Se_1, Se_2) \in B$ and $\Delta Se = Se_2 - Se_1$. Now the left hand inequality in (35) yields $q_{01} - q_{10} \leq Pr(Se_2 - Se_1)$, which together with (29) yields (34). Hence, by Lemma 2.9, we have $(Pr, Se_1, Se_2) \in B_{\leq}$ and thus $(Pr, \Delta Se) = (Pr, Se_2 - Se_1) \in C_{\leq}$. \square

PROOF OF LEMMA 2.11. Call D'_{\leq} the set claimed to equal D_{\leq} . By Lemma 2.9, we have $(Pr, Se_1) \in D_{\leq}$ iff there exists Se_2 with $(Pr, Se_1, Se_2) \in [0, 1]^3$ satisfying (30), (31), (32), and (34).

Let $(Pr, Se_1) \in D_{\leq}$ and let Se_2 be as just stated. Then (30) and (34) yield

$$\begin{aligned} Pr Se_1 &= \frac{1}{2} (Pr + Pr(Se_1 + Se_2 - 1) - Pr(Se_2 - Se_1)) \\ &\leq \frac{1}{2} (Pr + q_{11} - (q_{01} - q_{10})) = \frac{Pr + q_{1+} - q_{01}}{2} \end{aligned}$$

and (34) and $Se_2 \leq 1$ yield $Pr Se_1 = Pr Se_2 - Pr(Se_2 - Se_1) \leq Pr + q_{10} - q_{01}$. Combined with (31), we get (36). Hence $(Pr, Se_1) \in D'_{\leq}$.

Conversely, let $(Pr, Se_1) \in D'_{\leq}$. Then, since (36) implies (31), Lemma 2.6 yields $(Pr, Se_1) \in D$, so that there exists Se_2 with $(Pr, Se_1, Se_2) \in B$. By Lemma 2.4, this is equivalent to Se_2 fulfilling the conditions $Se_2 \in [0, 1]$ and (29)-(32), and we may assume that Se_2 has been chosen maximal with this property. Then at least one of the following four cases occurs, with each leading via (36) or trivially to $Pr(Se_2 - Se_1) \geq q_{01} - q_{10}$ and hence, using (29), to (34), proving $(Pr, Se_1) \in D_{\leq}$ as desired:

Case 1: $Se_2 = 1$. Then $Pr(Se_2 - Se_1) = Pr - Pr Se_1 \geq Pr - (Pr + q_{10} - q_{01}) = q_{01} - q_{10}$. Case 2: Equality holds on the right in (29). Case 3: Equality holds on the right in (30). Then

$$\begin{aligned} Pr(Se_2 - Se_1) &= Pr + Pr(Se_1 + Se_2 - 1) - 2 Pr Se_1 \\ &\geq Pr + q_{11} - (Pr + q_{1+} - q_{01}) = q_{01} - q_{10} \end{aligned}$$

Case 4: Equality holds on the right in (32). Then $Pr(Se_2 - Se_1) = Pr Se_2 - Pr Se_1 \geq q_{1+} - q_{1+} = q_{01} - q_{10}$. \square

PROOF OF LEMMA 2.12. Call E'_{\leq} the set claimed to equal E_{\leq} . By Lemma 2.9, we have $(Pr, Se_2) \in E_{\leq}$ iff there exists Se_1 with $(Pr, Se_1, Se_2) \in [0, 1]^3$ satisfying (30), (31), (32), and (34).

Let $(\Pr, \text{Se}_2) \in E_{\leq}$ and let Se_1 be as just stated. Then (30) and (34) yield

$$\begin{aligned}\Pr \text{Se}_2 &= \frac{1}{2}(\Pr + \Pr(\text{Se}_1 + \text{Se}_2 - 1) + \Pr(\text{Se}_2 - \text{Se}_1)) \\ &\geq \frac{1}{2}(\Pr - q_{00} + q_{01} - q_{10}) = \frac{\Pr + q_{01} - q_{+0}}{2}\end{aligned}$$

and (34) and $\Pr \text{Se}_1 \geq 0$ yield $\Pr \text{Se}_2 = \Pr(\text{Se}_2 - \text{Se}_1) + \Pr \text{Se}_1 \geq q_{01} - q_{10}$. Combined with (32), we get (37). Hence $(\Pr, \text{Se}_1) \in D'_{\leq}$.

Conversely, let $(\Pr, \text{Se}_2) \in E'_{\leq}$. Then, since (37) implies (32), Lemma 2.7 yields $(\Pr, \text{Se}_2) \in E$, so that there exists Se_1 with $(\Pr, \text{Se}_1, \text{Se}_2) \in B$. By Lemma 2.4, this is equivalent to Se_1 fulfilling the conditions $\text{Se}_1 \in [0, 1]$ and (29)-(32), and we may assume that Se_1 has been chosen minimal with this property. Then at least one of the following four cases occurs, with each leading via (37) or trivially to $\Pr(\text{Se}_2 - \text{Se}_1) \geq q_{01} - q_{10}$ and hence, using (29), to (34), proving $(\Pr, \text{Se}_2) \in E_{\leq}$ as desired:

Case 1: $\text{Se}_1 = 0$. Then $\Pr(\text{Se}_2 - \text{Se}_1) = \Pr \text{Se}_2 \geq q_{01} - q_{10}$. Case 2: Equality holds on the right in (29). Case 3: Equality holds on the left in (30). Then

$$\begin{aligned}\Pr(\text{Se}_2 - \text{Se}_1) &= -\Pr - \Pr(\text{Se}_1 + \text{Se}_2 - 1) + 2\Pr \text{Se}_2 \\ &\geq -\Pr + q_{00} + (\Pr + q_{01} - q_{+0}) = q_{01} - q_{10}\end{aligned}$$

Case 4: Equality holds on the left in (31). Then $\Pr(\text{Se}_2 - \text{Se}_1) = \Pr \text{Se}_2 - \Pr \text{Se}_1 \geq (\Pr - q_{+0}) - (\Pr - q_{0+}) = q_{01} - q_{10}$. \square

PROOF OF LEMMA 2.13. Call F'_{\leq} the interval claimed to equal F_{\leq} . By Lemma 2.10, we have $\Delta \text{Se} \in F_{\leq}$ iff there exists \Pr with $(\Pr, \Delta \text{Se}) \in [0, 1] \times [-1, 1]$ satisfying (35).

Let $\Delta \text{Se} \in F_{\leq}$ and let \Pr be as just stated. If $q_{01} - q_{10} > 0$, then (35) yields $\Pr > 0$ and hence $\Delta \text{Se} \geq (q_{01} - q_{10})/\Pr \geq q_{01} - q_{10}$. Hence always $\Delta \text{Se} \in F'_{\leq}$.

Conversely, let $\Delta \text{Se} \in F'_{\leq}$. If $q_{01} - q_{10} > 0$, then $\Pr := (q_{01} - q_{10})/\Delta \text{Se} \in [0, 1]$ satisfies (35). If $q_{01} - q_{10} \leq 0$, then $\Pr := 0$ satisfies (35). Hence $\Delta \text{Se} \in F_{\leq}$. \square

PROOF OF LEMMA 2.14. Call G'_{\leq} the interval claimed to equal G_{\leq} . By Lemma 2.11, we have $\text{Se}_1 \in G_{\leq}$ iff there exists \Pr with $(\Pr, \text{Se}_1) \in [0, 1]^2$ satisfying (36).

If $q_{01} - q_{10} \leq 0$, then $q_{+1} - q_{10} \leq q_{11}$ and hence $G'_{\leq} = [0, 1]$; and given $\text{Se}_1 \in [0, 1]$, we may put $\Pr := 0$ to satisfy (36), so that also $G_{\leq} = [0, 1]$.

So let $q_{01} - q_{10} > 0$ for the rest of this proof. The three functions $f_i : [0, 1] \rightarrow \mathbb{R}$ defined by

$$f_1(x) := \frac{q_{1+}}{x} \quad f_2(x) := \frac{1}{2} + \frac{q_{1+} - q_{01}}{2x} \quad f_3(x) := 1 - \frac{q_{01} - q_{10}}{x}$$

are continuous and monotone with $\lim_{x \rightarrow 0} f_3(x) = -\infty$, so that their pointwise infimum $f := f_1 \wedge f_2 \wedge f_3$ attains its maximal value at $\Pr_1 := 1$ or at some $x \in]0, 1]$ satisfying $f_i(x) = f_j(x)$ with $i < j$. The latter three equations have the unique solutions $\Pr_{12} := q_{1+} + q_{01}$, $\Pr_{13} := q_{+1}$, $\Pr_{23} := q_{+1} - q_{10}$, each strictly positive by $q_{01} - q_{10} > 0$, and we get

$$\begin{aligned} f(\Pr_1) &= q_{1+} \wedge \frac{1 + q_{1+} - q_{01}}{2} \wedge (1 + q_{10} - q_{01}) = q_{1+} \\ f(\Pr_{12}) &= \frac{q_{1+}}{q_{1+} + q_{01}} \wedge \left(1 - \frac{q_{01} - q_{10}}{q_{1+} + q_{01}}\right) = \frac{q_{1+}}{q_{1+} + q_{01}} \\ f(\Pr_{13}) &= \frac{q_{1+}}{q_{+1}} \wedge \left(\frac{1}{2} + \frac{q_{1+} - q_{01}}{2q_{+1}}\right) = \frac{q_{1+} + q_{11}}{2q_{+1}} \\ f(\Pr_{23}) &= \frac{q_{1+}}{q_{+1} - q_{10}} \wedge \left(1 - \frac{q_{01} - q_{10}}{q_{+1} - q_{10}}\right) = \frac{q_{11}}{q_{+1} - q_{10}} \end{aligned}$$

We have $f(\Pr_1) \leq f(\Pr_{12})$ since $q_{1+} + q_{01} \leq 1$. Writing here $a \sim b$ to indicate that $ab > 0$ or $a = b = 0$ holds, clearing fractions yields

$$\begin{aligned} f(\Pr_{12}) - f(\Pr_{13}) &\sim 2q_{+1}q_{1+} - (q_{1+} + q_{01})(q_{1+} + q_{11}) = q_{01}(q_{01} - q_{1+}) \\ f(\Pr_{23}) - f(\Pr_{13}) &\sim 2q_{+1}q_{11} - (q_{+1} - q_{10})(q_{1+} + q_{11}) = q_{01}(q_{1+} - q_{01}) \end{aligned}$$

Hence $\max f = f(\Pr_{12}) \vee f(\Pr_{23})$, namely attained at \Pr_{12} if $q_{01} \geq q_{1+}$ and at \Pr_{23} if $q_{01} \leq q_{1+}$.

Now let $\text{Se}_1 \in G_{\leq}$ and let $\Pr \in [0, 1]$ with (36). Then in particular $\Pr \text{Se}_1 \leq \Pr + q_{10} - q_{01}$ and thus $\Pr > 0$, using $q_{01} - q_{10} > 0$. Thus (36) yields $\text{Se}_1 \leq f(\Pr) \leq \max f$ and thus $\text{Se}_1 \in G'_{\leq}$.

Conversely, let $\text{Se}_1 \in G'_{\leq}$. Then $\text{Se}_1 \leq \max f$ and thus, by $\lim_{x \rightarrow 0} f(x) = -\infty$ and continuity of f , there is a $\Pr \in]0, 1]$ with $f(\Pr) = \text{Se}_1$, yielding $\Pr \text{Se}_1 = \Pr f(\Pr) = \text{R.H.S.(36)} \geq \text{L.H.S.(36)}$, with the last inequality due to $\Pr \leq 1$ and $q \in \text{prob}(\{0, 1\}^2)$, so that (36) holds and hence $\text{Se}_1 \in G_{\leq}$. \square

PROOF OF LEMMA 2.15. Very similar to the above proof of Lemma 2.14, with the following differences: Use Lemma 2.12 in place of Lemma 2.11. After again restricting attention to the main case where $q_{01} - q_{10} > 0$, define now

$$f_1(x) := 1 - \frac{q_{+0}}{x} \quad f_2(x) := \frac{1}{2} + \frac{q_{01} - q_{+0}}{2x} \quad f_3(x) := \frac{q_{01} - q_{10}}{x}$$

and observe that $f := f_1 \vee f_2 \vee f_3$ is minimized over $]0, 1]$ at one of $\Pr_1 := 1$, $\Pr_{12} := q_{+0} + q_{01}$, $\Pr_{13} := q_{0+}$, $\Pr_{23} := q_{0+} - q_{10}$. After computing $f(\Pr_1) = q_{+1}$, $f(\Pr_{12}) = \frac{q_{01}}{q_{+0} + q_{01}}$, $f(\Pr_{13}) = \frac{2q_{01} - q_{10}}{2q_{0+}}$, $f(\Pr_{23}) = \frac{q_{01} - q_{10}}{q_{0+} - q_{10}}$, one observes $f(\Pr_1) \geq f(\Pr_{12})$ and

$$f(\Pr_{12}) - f(\Pr_{13}) \sim q_{10}(q_{+0} - q_{01}) \sim f(\Pr_{13}) - f(\Pr_{23})$$

Hence $\min f = f(\Pr_{12}) \wedge f(\Pr_{23})$. \square

PROOF OF LEMMA 2.16. Call I'_{\leq} the interval claimed to equal I_{\leq} . By Lemma 2.10, we have $\Pr \in I_{\leq}$ iff there exists ΔSe with $(\Pr, \Delta Se) \in [0, 1] \times [-1, 1]$ satisfying (35).

Let $\Pr \in I_{\leq}$ and let ΔSe be as just stated. If $q_{01} - q_{10} = 0$, then $I'_{\leq} = [0, 1]$ and hence $\Pr \in I'_{\leq}$. If $q_{01} - q_{10} > 0$, then (35) implies $\Delta Se > 0$ and hence $\Pr \geq (q_{01} - q_{10})/\Delta Se \geq q_{01} - q_{10}$ and thus again $\Pr \in I'_{\leq}$. If $q_{01} - q_{10} < 0$, then either $q_{01} - q_{10} + 1 - \Pr \geq 0$ and then $\Pr \leq 1 - (q_{10} - q_{01})^+$, or $q_{01} - q_{10} + 1 - \Pr < 0$ and then (35) yields $\Delta Se < 0$ and thus $\Pr \leq (q_{01} - q_{10})/\Delta Se \leq q_{10} - q_{01}$, so that $\Pr \in I'_{\leq}$ also in this case.

Conversely, let $\Pr \in I'_{\leq}$. If $q_{01} - q_{10} \leq 0$, then either $q_{01} - q_{10} + 1 - \Pr \geq 0$ and then $\Delta Se := 0$ satisfies (35), or $q_{01} - q_{10} + 1 - \Pr < 0$ and then $\Pr \in I'_{\leq}$ yields $\Pr \leq q_{10} - q_{01}$ so that $\Delta Se := -1$ satisfies (35). If $q_{01} - q_{10} > 0$, then $\Delta Se := (q_{01} - q_{10})/\Pr \in]0, 1]$ satisfies (35). Hence $\Pr \in I_{\leq}$ in every case. \square

4. The remaining proofs. Below we prove Theorems 1.1 and Theorem 1.2 by applying the rather general and trivial Lemmas 4.1 and 4.2 together with the special Lemmas 2.3, 2.10, and 2.12. We then deduce Theorem 1.2 from Theorem 1.3.

LEMMA 4.1. *Let $\mathcal{P} = (P_{\vartheta} : \vartheta \in \Theta)$ and $\mathcal{Q} = (Q_{\eta} : \eta \in H)$ be experiments on the same sample space \mathcal{X} , with parameters of interest $\kappa : \Theta \rightarrow \bar{\mathbb{R}}$ and $\lambda : H \rightarrow \bar{\mathbb{R}}$. Let $\beta \in [0, 1]$.*

A. *Assume the implication*

$$(44) \quad \eta \in H \Rightarrow \exists \vartheta \in \Theta \text{ with } P_{\vartheta} = Q_{\eta} \text{ and } \kappa(\vartheta) \leq \lambda(\eta)$$

Then every lower β -confidence bound for (\mathcal{P}, κ) is also one for (\mathcal{Q}, λ) .

B. *Assume the implication*

$$(45) \quad \eta \in H \Rightarrow \exists \vartheta \in \Theta \text{ with } P_{\vartheta} = Q_{\eta} \text{ and } \kappa(\vartheta) \geq \lambda(\eta)$$

and let $\underline{\kappa}$ and $\underline{\lambda}$ be both lower β -confidence bounds for (\mathcal{P}, κ) and for (\mathcal{Q}, λ) , with $\underline{\lambda}$ worse than $\underline{\kappa}$ for (\mathcal{P}, κ) . Then $\underline{\lambda}$ is also worse than $\underline{\kappa}$ for (\mathcal{Q}, λ) .

Analogously for upper confidence bounds, with “ \leq ” and “ \geq ” interchanged.

PROOF. A. Let $\underline{\kappa}$ be a lower β -confidence bound for (\mathcal{P}, κ) and let $\eta \in H$. With ϑ from (44) then $Q_{\eta}(\underline{\kappa} \leq \lambda(\eta)) = P_{\vartheta}(\underline{\kappa} \leq \lambda(\eta)) \geq P_{\vartheta}(\underline{\kappa} \leq \kappa(\vartheta)) \geq \beta$.

B. Let $\eta \in H$ and $t < \lambda(\eta)$. With ϑ from (45) we then have $t < \kappa(\vartheta)$ and hence $Q_{\eta}(\underline{\lambda} \geq t) = P_{\vartheta}(\underline{\lambda} \geq t) \leq P_{\vartheta}(\underline{\kappa} \geq t) = Q_{\eta}(\underline{\kappa} \geq t)$. \square

Below, a *natural exponential family*, or *NEF* for short, is any statistical model $\mathcal{Q} = (Q_\eta : \eta \in H)$ such that, for some $k \in \mathbb{N}$ and some measure ν on \mathbb{R}^k , we have $H \subseteq \mathbb{R}^k$ and, for each $\eta \in H$, Q_η is a law on \mathbb{R}^k with a ν -density proportional to $y \mapsto \exp(\sum_{i=1}^k \eta_i y_i)$.

LEMMA 4.2. *Let $\mathcal{Q} = (Q_\eta : \eta \in H)$ be a NEF with H open and nonempty. Let $\lambda : H \rightarrow \overline{\mathbb{R}}$ be lower semicontinuous and let $\underline{\lambda}$ and $\overline{\lambda}$ be equivalent lower confidence bounds for (\mathcal{Q}, λ) . Then $\underline{\lambda} \wedge \sup \lambda(H) = \overline{\lambda} \wedge \sup \lambda(H)$ \mathcal{Q} -a.s.*

PROOF. The equivalence assumption yields

$$(46) \quad Q_\eta(\lambda > t) = Q_\eta(\underline{\lambda} > t) \quad \text{if } \eta \in H \text{ and } t \in [-\infty, \lambda(\eta)[$$

For fixed $t \in \mathbb{R}$ with $t < \sup \lambda(H)$, the subfamily $(Q_\eta : \eta \in H, \lambda(\eta) > t)$ is again a NEF with nonempty open parameter space, hence complete in the sense of Lehmann-Scheffé, so that (46) yields $\{\underline{\lambda} > t\} = \{\overline{\lambda} > t\}$ \mathcal{Q} -a.s. Hence

$$\{\underline{\lambda} \wedge \sup \lambda(H) \neq \overline{\lambda} \wedge \sup \lambda(H)\} = \bigcup_{t \in \mathbb{Q}, t < \sup \lambda(H)} \{\underline{\lambda} \leq t < \overline{\lambda}\} \cup \{\overline{\lambda} \leq t < \underline{\lambda}\}$$

is a \mathcal{Q} -null set. \square

PROOF OF THEOREM 1.1. We first check the applicability of Lemma 4.1 to some pairs of estimation problems. Recall μ and P_ϑ from (3) and (4).

The problems $(\mathcal{M}, (8))$ and $(\mathcal{P}_2, (9))$, in this order but also in the reversed one, fulfill the assumptions of Lemma 4.1 A and B: For the stated order, given $\vartheta = (\pi, \chi) \in \Theta_2$, put $q := \mu(\vartheta) \in \text{prob}(\{0, 1\}^2)$, and observe that then $M_{n,q} = P_\vartheta$ and R.H.S.(8) = R.H.S.(9) by Lemma 2.3(27). For the reversed order, given $q \in \text{prob}(\{0, 1\}^2)$, choose $\vartheta \in \Theta_2$ with $\mu(\vartheta) = q$ using the nonemptiness claim of Lemma 2.3, and finish as in the preceding sentence.

The problems $(\mathcal{P}_2, (9))$ and $(\mathcal{P}_{2,\leq}, (10))$ fulfill the assumptions of Lemma 4.1 A, since for $\vartheta \in \Theta_{2,\leq}$, we also have $\vartheta \in \Theta_2$ and $\text{R.H.S.}(9) \leq \text{R.H.S.}(10)$.

The problems $(\mathcal{P}_{2,\leq}, (10))$ and $(\mathcal{M}, (8))$ fulfill the assumptions of Lemma 4.1 A and B: Given $q \in \text{prob}(\{0, 1\}^2)$, Lemma 2.10 with $\Pr = 1$ yields a $\vartheta = (\pi, \chi) \in \Theta_{2,\leq}$ with $\mu(\vartheta) = q$, so $P_\vartheta = M_{n,q}$, and $\text{R.H.S.}(10) = \text{R.H.S.}(8)$.

Applying now Lemma 4.1 several times yields parts A and B of the theorem. The subclaim of Part C referring only to $(\mathcal{M}, (8))$ and $(\mathcal{P}_2, (9))$ follows directly from Parts A and B, as “ $\underline{\Delta}$ strictly worse than $\overline{\Delta}$ ” is equivalent to “ $\underline{\Delta}$ worse than $\overline{\Delta}$, and not $\overline{\Delta}$ worse than $\underline{\Delta}$ ”.

Finally, let $\underline{\Delta}$ be admissible as a lower β -confidence bound for $(\mathcal{M}, (8))$. By Part A, $\underline{\Delta}$ is also a β -confidence bound for $(\mathcal{P}_{2,\leq}, (10))$. Let $\tilde{\Delta}$ be a better β -confidence bound for $(\mathcal{P}_{2,\leq}, (10))$. We have to show that $\tilde{\Delta}$ is equivalent to $\underline{\Delta}$ for $(\mathcal{P}_{2,\leq}, (10))$. By Part B, $\tilde{\Delta}$ is better than $\underline{\Delta}$ also for $(\mathcal{M}, (8))$ and hence, by the assumed admissibility, in fact equivalent to $\underline{\Delta}$ for $(\mathcal{M}, (8))$. With a view towards applying Lemma 4.2, we put $H := \{\eta \in]-\infty, 0]^3 : \sum_{i=1}^3 e^{\eta_i} < 1\}$, define a function $\tau : H \rightarrow \text{prob}(\{0, 1\}^2)$ by $\tau_{00}(\eta) := e^{\eta_1}$, $\tau_{01}(\eta) := e^{\eta_2}$, $\tau_{10}(\eta) := e^{\eta_3}$, and $\tau_{11}(\eta) := 1 - \sum_{i=1}^3 e^{\eta_i}$ for $\eta \in H$, and put $\mathcal{Q} := \mathcal{M} \circ \tau$, that is, $\mathcal{Q} = (Q_\eta : \eta \in H)$ with $Q_\eta = M_{n,\tau(\eta)}$. Let κ denote the function (8) and let $\lambda := \kappa \circ \tau$ so that, writing $\text{Prob}(\mathcal{X})$ for the set of all laws on $\mathcal{X} := \{k \in \mathbb{N}_0^{\{0,1\}^2} : k_{++} = n\}$, the diagram

$$\begin{array}{ccccc} & & H & & \\ & \swarrow \tau & \downarrow \tau & \searrow \varphi & \\ \mathbb{R} & \xleftarrow[\kappa]{} & \text{prob}(\{0, 1\}^2) & \xrightarrow[\mathcal{M}]{} & \text{Prob}(\mathcal{X}) \end{array}$$

commutes. Then, trivially, $\lambda := \underline{\Delta}$ and $\lambda := \tilde{\Delta}$ are equivalent lower confidence bounds for (\mathcal{Q}, λ) . Now Lemma 4.2 applies and yields $\underline{\Delta} \wedge 1 = \tilde{\Delta} \wedge 1$ everywhere on \mathcal{X} and hence, as (10) is $[-1, 1]$ -valued, the wanted equivalence. \square

PROOF OF THEOREM 1.2. The problems $(\mathcal{M}, (13))$ and $(\mathcal{P}_{2,\leq}, (14))$ fulfill the assumptions of the “upper” version of Lemma 4.1 A, since for $\vartheta \in \Theta_{2,\leq}$ and $q := \mu(\vartheta)$, we have $R.H.S.(13) \geq R.H.S.(14)$ by Lemma 2.14. The problems $(\mathcal{P}_{2,\leq}, (14))$ and $(\mathcal{M}, (13))$ fulfill the assumptions of the “upper” version of Lemma 4.1 A and B, since for $q \in \text{prob}(\{0, 1\}^2)$, Lemma 2.14 yields a $\vartheta \in \Theta_{2,\leq}$ with $\mu(\vartheta) = q$ and $R.H.S.(14) = R.H.S.(13)$. Hence Lemma 4.1 yields parts A and B of the theorem.

To prove Part C, we can proceed as in the last paragraph of our proof of Theorem 1.1, with the following changes: Given now \bar{S} and \tilde{S} , we let κ denote the function (13). Then Lemma 4.2 applies with $\underline{\lambda} := -\bar{S}$ and $\tilde{\lambda} := -\tilde{S}$ to yield $\bar{S} \vee 0 = \tilde{S} \vee 0$. Here $-\kappa \circ \eta$ is indeed lower semicontinuous, but one could also replace H by $\{\eta \in H : \eta_2 > \eta_3\}$; then $-\kappa \circ \eta$ would be continuous. \square

PROOF OF THEOREM 1.3. The function (16) is an upper β -confidence bound in the quadrinomial model $\mathcal{M} := (M_{n,q} : q \in \text{prob}(\{0, 1\}^2))$ and for the parameter (13) from Theorem 1.2, since for $q \in \text{prob}(\{0, 1\}^2)$, conditioning

on the upper left corner of our 2×2 table yields

$$\begin{aligned} & M_{n,q} \left(\left\{ k \in \mathbb{N}_0^{\{0,1\}^2} : k_{++} = n, u(k_{10}, k_{01}, k_{11}) \geq \text{R.H.S.(13)} \right\} \right) \\ &= \sum_{m=0}^n b_{n,q_{00}}(n-m) M_{m,p} \left(\left\{ j \in \mathbb{N}_0^{\{1,2,3\}} : j_+ = m, u(j) \geq \text{R.H.S.(15)} \right\} \right) \\ &\geq \beta \end{aligned}$$

with $b_{n,q_{00}}$ denoting a binomial density, and with $p \in \text{prob}(\{1, 2, 3\})$ defined by $p := (1 - q_{00})^{-1}(q_{10}, q_{01}, q_{11})$ if $q_{00} < 1$, and $p := (0, 0, 1)$ if $q_{00} = 1$. Hence the claim follows from Theorem 1.2 A. \square

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UNIVERSITÄT TRIER
FACHBEREICH IV - MATHEMATIK
54286 TRIER
GERMANY
E-MAIL: mattner@uni-trier.de

UNIVERSITÄTSKLINIKUM DER PRIVATEN
UNIVERSITÄT WITTEN-HERDECKE,
CAMPUS KÖLN-MERHEIM,
INSTITUT FÜR HYGIENE
OSTMERheimer STRASSE 200
51109 KÖLN
GERMANY
E-MAIL: mattnerf@kliniken-koeln.de